STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 168496

TO:	From:
David Lukton **Location: REM-3B75/3C18** **Art Unit: 1654** **Monday, August 29, 2005** **Case Serial Number: 09/600659**	**Edward Hart** **Location: Biotech-Chem Library** **REM-1A55** **Phone: 571-272-2512** **edward.hart@uspto.gov**

Search Notes

Examiner Lukton,

Here are the results of the search you requested.

Please feel free to contact me if you have any questions.

Edward Hart

ACCESS DB # _____

PLEASE PRINT CLEARLY

SEARCH REQUEST FORM
(STIC)

Requestor's Name: David Lukton Examiner number: 71263 Date: 7/6/05

Art Unit: 1654 Phone number: 571-272-0952 Serial Number: 09/600659

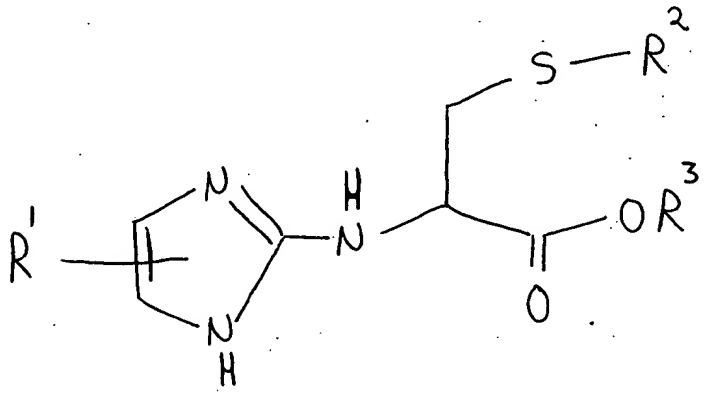
Mail Box: 3-C-18 Examiner Rm: 3-B-75 Results format: paper

* * * * * * * *

Title: A PHARMACEUTICAL FORMULATION CONTAINING AN INHIBITOR OF CARBOXYPEPTIDASE U AND A THROMBIN INHIBITOR

Applicants: ABRAHAMSSON, TOMMY; NERME, VIVECA; POLLA, MAGNUS

Earliest Priority Date: 5/3/99



R^1 = amino or alkylamino or amidino or guanidino;

R^2 = hydrogen or acyl;

R^3 is anything;

****

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: 8/4/05

Date Completed: _____

Searcher Prep & Review Time: _____

Online Time: _____

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

_____ Structure (#)

_____ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

(STN) _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

___ In-house sequence systems

___ Commercial ___ Oligomer ___ Score/Length

___ Interference ___ SPDI ___ Encode/Transl

_____ Other (specify)

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FILE 'HCAPLUS' ENTERED AT 15:33:36 ON 29 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 29 Aug 2005  VOL 143 ISS 10
FILE LAST UPDATED: 28 Aug 2005  (20050828/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L6                STR
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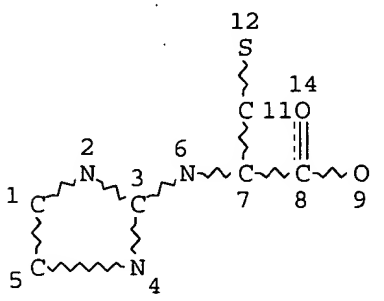


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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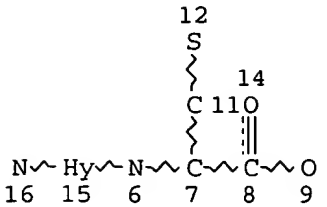


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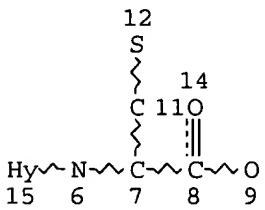


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STEREO ATTRIBUTES: NONE
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L21           34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20
L22           30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 AND PD<=MAY 3, 1999


=> d ibib abs hitstr l22 tot

L22  ANSWER 1 OF 30  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1999:318208  HCAPLUS
DOCUMENT NUMBER:          131:166490
TITLE:                    Root-exudated compounds as conjugation partners of
                          pesticides in the rhizosphere
AUTHOR(S):                Schneider, R. J.
CORPORATE SOURCE:         Institut fur Agrikulturchemie Universitat Bonn, Bonn,
                          D - 53115, Germany
SOURCE:                   Pflanzenernaehrung, Wurzelleistung und Exsudation,
                          Borkheider Seminar zur Oekophysiologie des
```

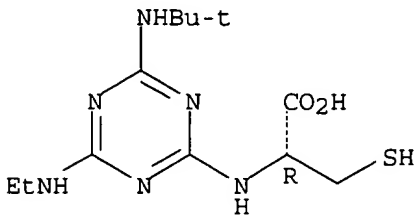
Wurzelraumes, 8th, Schmerwitz, Germany, Sept. 22-24, 1997 (**1998**), Meeting Date 1997, 213-220.
Editor(s): Merbach, Wolfgang. Teubner: Stuttgart, Germany.
CODEN: 67RDAF
DOCUMENT TYPE: Conference
LANGUAGE: German

AB The formation of bound residues from pesticides in soil is still poorly understood. We assume that low mol. substances exudated from the roots of living plants are potential reaction partners for xenobiotic mols. in the rhizosphere. A reaction of pesticides with low-mol. substances as amino acids, carboxylic acids and carbohydrates should be kinetically favored in regard to the relatively inert central regions of humic substances. Possible conjugates of the terbuthylazine have been postulated and synthesized. First results on the occurrence of these metabolites are presented.

IT **239092-58-1P**
RL: AGR (Agricultural use); FMU (Formation, unclassified); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)
(preparation as model for pesticide conjugates with rhizospheric root exudates)

RN 239092-58-1 HCAPLUS
CN L-Cysteine, N-[4-[(1,1-dimethylethyl)amino]-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:471284 HCAPLUS
DOCUMENT NUMBER: 129:171820
TITLE: The metabolism of atrazine and related 2-chloro-4,6-bis(alkylamino)-s-triazines in plants
AUTHOR(S): Lamoureux, Gerald L.; Simoneaux, Bruce; Larson, John
CORPORATE SOURCE: Biosciences Research Laboratory, ARS, USDA, State University Station, Fargo, ND, 58105-5674, USA
SOURCE: ACS Symposium Series (**1998**), 683(Triazine Herbicides: Risk Assessment), 60-81
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

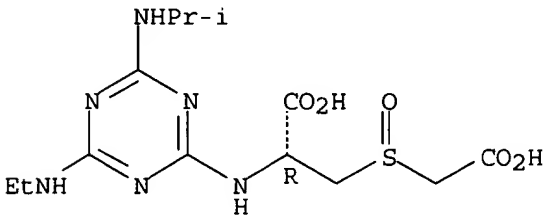
AB The metabolism of atrazine and related 2-chloro-4,6-bis(alkylamino)-s-triazine herbicides in plants is summarized and the structures of 13 metabolites recently identified from mature plants grown in the field are reported. The 2-chloro-4,6-bis(alkylamino)-s-triazines are initially metabolized in

plants by 3 competing reactions: hydrolytic dehalogenation, N-dealkylation, and glutathione (GSH) conjugation. Metabolites produced by N-dealkylation can be further metabolized by hydrolytic dehalogenation or GSH conjugation, those produced by hydrolytic dehalogenation can be further metabolized by N-dealkylation and it is proposed that those from the GSH conjugation pathway may slowly become hydroxylated at the 2-position of the triazine ring. Ten metabolites of atrazine have been identified from the N-dealkylation and hydroxylation pathways and 14 have been identified from the GSH conjugation pathway. Three addnl. metabolites that have an amino function on the 2-position of the triazine ring have been identified, but their route of formation is uncertain.

IT **211558-12-2 211558-13-3 211558-14-4**
211558-15-5 211558-16-6
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(atrazine metabolite in sugarcane)

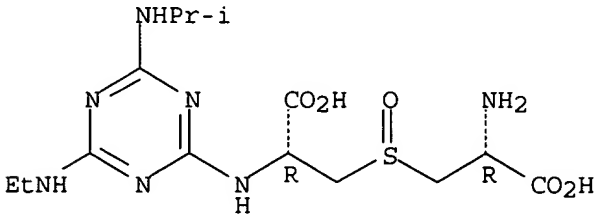
RN 211558-12-2 HCAPLUS
CN L-Alanine, 3-[(carboxymethyl)sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



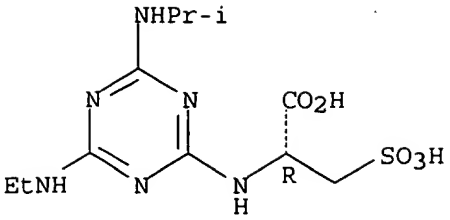
RN 211558-13-3 HCAPLUS
CN L-Alanine, 3-[[(2R)-2-amino-2-carboxyethyl]sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



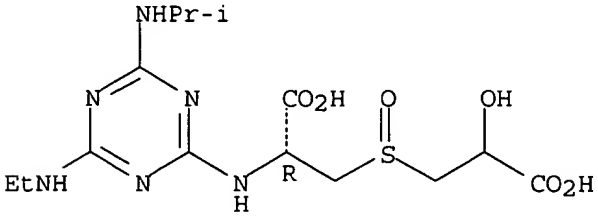
RN 211558-14-4 HCAPLUS
CN L-Alanine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]-3-sulfo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



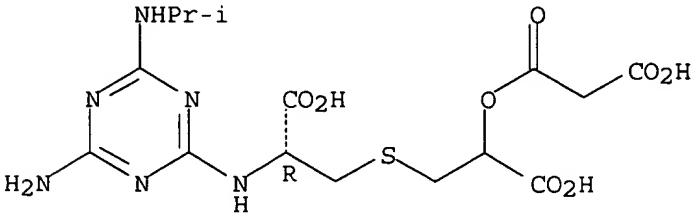
RN 211558-15-5 HCAPLUS
CN L-Alanine, 3-[(2-carboxy-2-hydroxyethyl)sulfinyl]-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 211558-16-6 HCAPLUS
CN Propanedioic acid, mono[2-[[(2R)-2-[[4-amino-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]-2-carboxyethyl]thio]-1-carboxyethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:635209 HCAPLUS
DOCUMENT NUMBER: 125:250609
TITLE: Magenta recording fluids for ink-jet recording with good water resistance
INVENTOR(S): Satoh, Nobuyoshi; Hirasa, Takashi; Murata, Yukichi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9626985	A1	19960906	WO 1995-JP336	19950302 <--
W: US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 758672	A1	19970219	EP 1995-910729	19950302 <--
EP 758672	B1	20020731		
R: DE, GB				
US 5713992	A	19980203	US 1997-732451	19970113 <--
PRIORITY APPLN. INFO.:			WO 1995-JP336 W	19950302
OTHER SOURCE(S):	MARPAT 125:250609			

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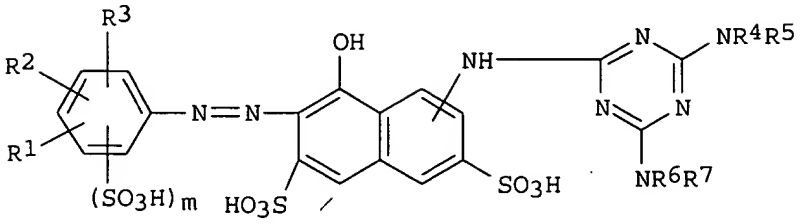

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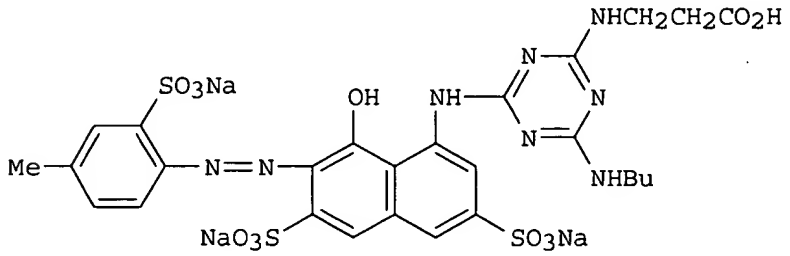


II

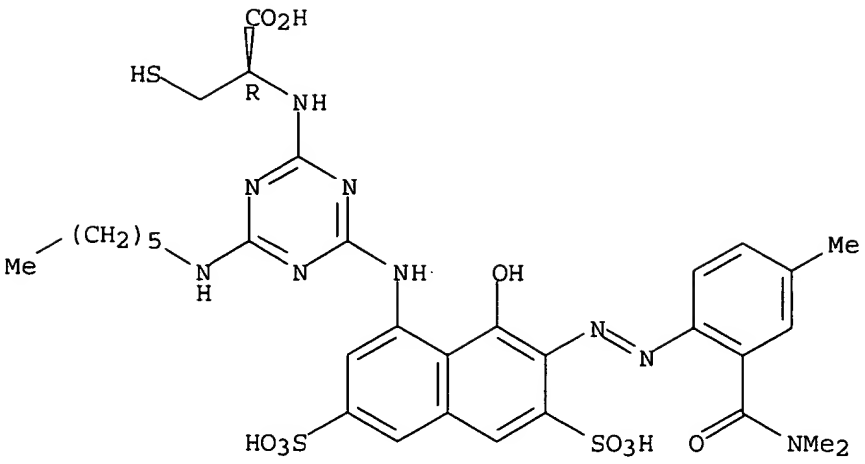
AB The title fluids comprise an aqueous medium and ≥1 monoazo dye I in free-acid form [R1-3 = H, (un)substituted C1-C9 alkyl, alkoxy, halogen, OH, (un)substituted carbamoyl, sulfamonyl, amino, nitro, sulfonic ester, sulfonyl, COOH, or carboxylic ester group; m =0-2; R4-7 = H, C1-C18 alkyl, alkenyl, aryl, aralkyl, alicyclic or heterocyclic group, provided that all of the above non-H groups may be substituted and that ≥1 of R4-7 is substituted by COOH]. A fluid from diethylene glycol 10, iso-PrOH 3, II 3, and water to 100 parts, adjusted to pH 9 by aqueous ammonia provided light- and wetfast jet prints on copying paper.

IT **182307-47-7**
RL: TEM (Technical or engineered material use); USES (Uses)
(magenta recording fluids for ink-jet recording with good water resistance)

RN 182307-47-7 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-3,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



●2 Na

L22 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:169303 HCAPLUS
DOCUMENT NUMBER: 124:263652
TITLE: Water-based black recording liquids containing azo dyes
INVENTOR(S): Sano, Hideo; Yamada, Masahiro; Nishimura, Tooru; Takimoto, Hiroshi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07331145	A2	19951219	JP 1994-125100	19940607 <--
JP 3371542	B2	20030127		

PRIORITY APPLN. INFO.: JP 1994-125100 19940607
OTHER SOURCE(S): MARPAT 124:263652
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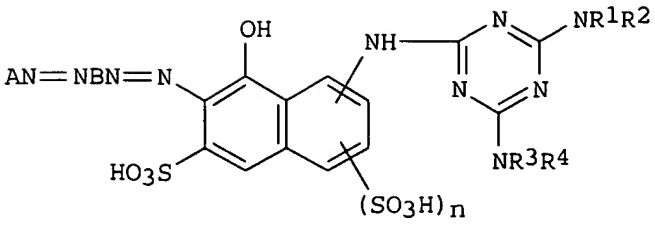

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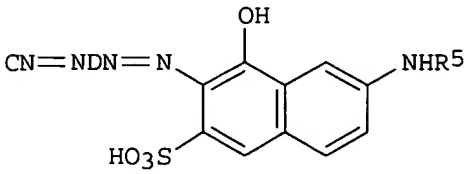


II

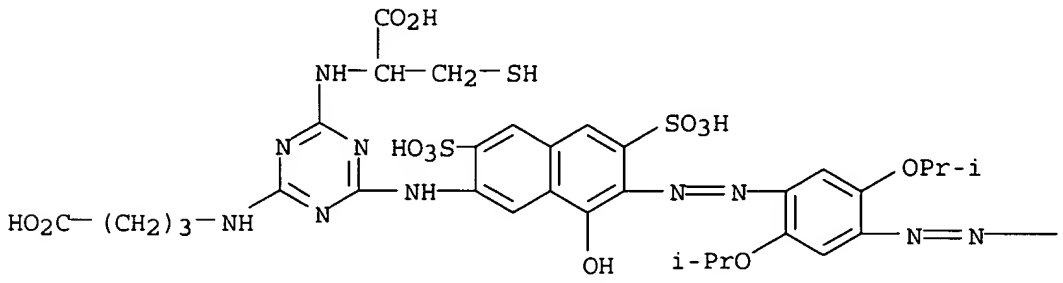
AB Title liqs., useful for ink-jet printing black inks, etc., contain aqueous medium and ≥1 I-type azo dye and ≥1 II-type azo dyes [as free acids; A, C = (substituted) Ph, (substituted) naphthyl; B, D = (substituted) phenylene, (substituted) naphthylene; R1-5 = H, C1-18 alkyl, C1-18 alkenyl, aryl, aralkyl, cycloalkyl, heterocycle; which may be substituted; ≥1 R1-4 are carboxyl-substituted; n = 0-1]. The liqs. may comprise water 35-93, water-soluble organic solvents 5-50, and the dyes 2-8%.

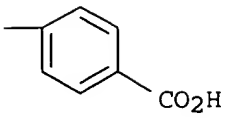
IT **175466-11-2**
RL: TEM (Technical or engineered material use); USES (Uses)
(black water-based jet printing inks containing disazo dyes)

RN 175466-11-2 HCAPLUS

CN Benzoic acid, 4-[[4-[[7-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A





L22 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:35311 HCAPLUS
DOCUMENT NUMBER: 124:90619
TITLE: Ink-jet printing liquids containing triazine-substituted azo magenta dyes
INVENTOR(S): Sano, Hideo; Murata, Jukichi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07278478	A2	19951024	JP 1994-72186	19940411 <--
JP 3440544	B2	20030825		
PRIORITY APPLN. INFO.:			JP 1994-72186	19940411

OTHER SOURCE(S): MARPAT 124:90619
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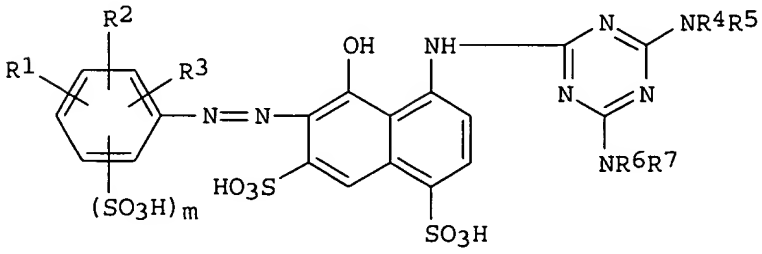


I

AB Title inks contain water-based mediums and I [R1-R3 = C1-9 (substituted) alkyl, C1-9 alkoxy, halo, H, OH, (substituted) carbamoyl, (substituted) sulfamoyl, (substituted) amino, NO2, sulfonate ester, SO2, CO2H, carboxylate ester; R4-R7 = H, C1-18 (substituted) alkyl, (substituted) alkenyl, aryl, aralkyl, alicyclic or heterocyclic group; m = 0-2]. The

inks provide magenta printed image with high color d., good light and water resistance. Thus, an ink containing I (R1 = p-Me; o-SO3Na; R2-R6 = H; R5 = C2H4CO2H; R7 = Bu; Na salt), diethylene glycol, iso-Pr alc., and water was subjected to ink-jet printing onto electrophotog. printing paper.

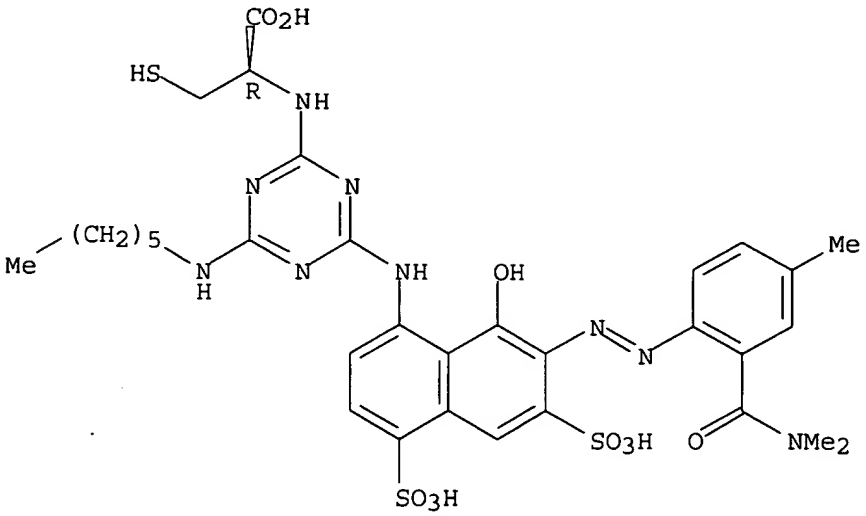
IT **172852-74-3**
RL: TEM (Technical or engineered material use); USES (Uses)
(dyes; water-based jet-printing inks containing triazine-substituted magenta azo dyes)

RN 172852-74-3 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-4,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, dilithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 2-A

●2 Li

L22 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:867632 HCAPLUS
DOCUMENT NUMBER: 123:260079
TITLE: Jet-printing and writing inks
INVENTOR(S): Sano, Hideo; Murata, Yukichi; Nishimura, Toru; Yamada, Masahiro; Takimoto, Hiroshi; Sato, Nobuyoshi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
SOURCE: Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

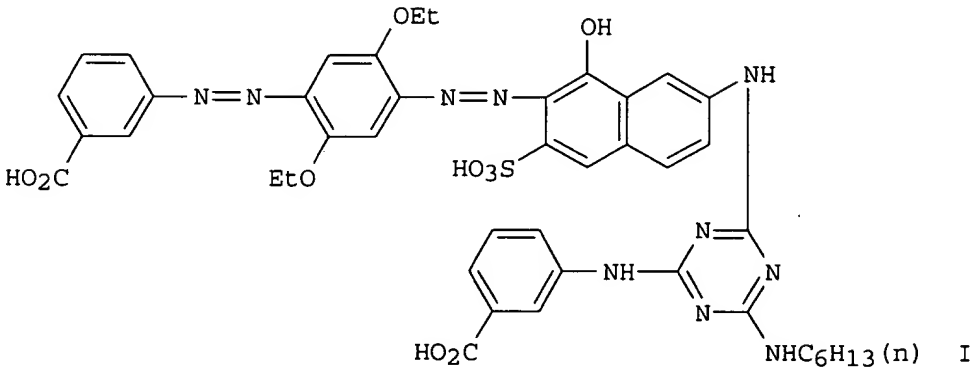
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 656407	A2	19950607	EP 1994-118779	19941129 <--
EP 656407	A3	19960710		
EP 656407	B1	19990303		
R: DE, FR, GB				
JP 07196967	A2	19950801	JP 1994-271413	19941104 <--
JP 3451755	B2	20030929		
JP 07207203	A2	19950808	JP 1994-271415	19941104 <--
JP 3484581	B2	20040106		
JP 07207204	A2	19950808	JP 1994-271416	19941104 <--
JP 3467533	B2	20031117		
JP 08113742	A2	19960507	JP 1994-271414	19941104 <--
JP 3428178	B2	20030722		

PRIORITY APPLN. INFO.:

JP 1993-298186	A	19931129
JP 1993-301925	A	19931201
JP 1993-301927	A	19931201
JP 1994-202056	A	19940826

OTHER SOURCE(S): MARPAT 123:260079

GI



I

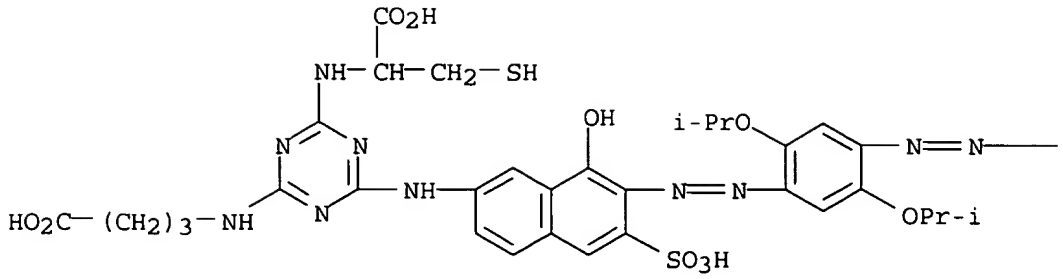
AB Storage-stable title inks that provide high-d. black images with good color tone and light and water resistance contain ≥1 dye selected from a series of dis- and trisazo acid dyes, some of which contain triazine groups. A typical aqueous ink with pH 9 contained diethylene glycol 10, iso-PrOH 3, and disazo dye I 3 parts.

IT **169195-81-7 169195-92-0**
RL: TEM (Technical or engineered material use); USES (Uses)
(dye; storage-stable jet-printing and writing inks containing acid dis- or trisazo dyes and providing high-d. black images with good color tone and light and water resistance)

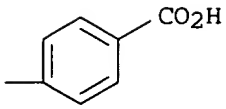
RN 169195-81-7 HCAPLUS

CN Benzoic acid, 4-[[4-[[7-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

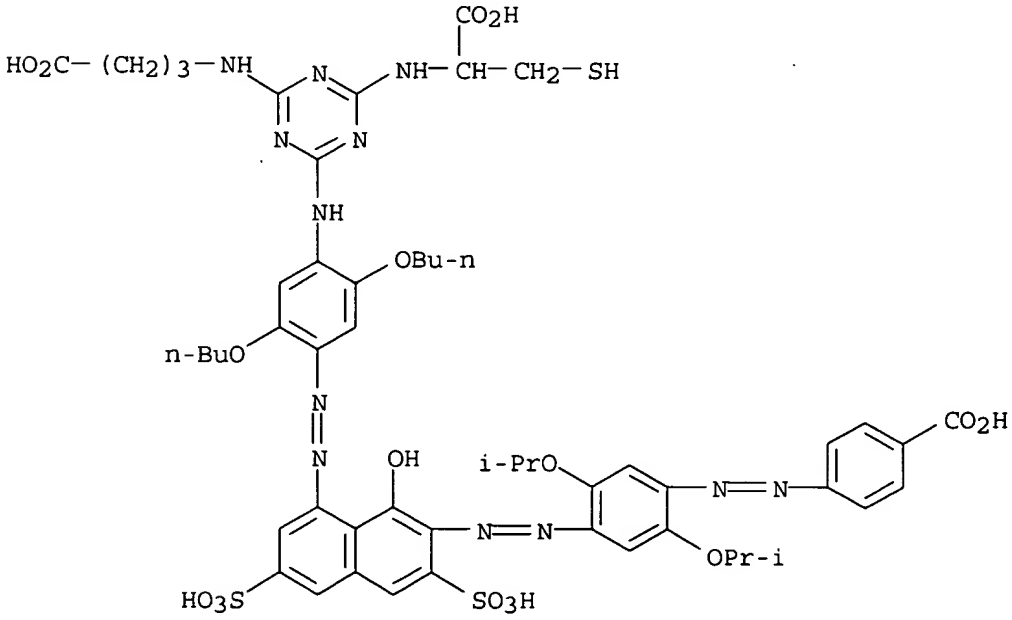
PAGE 1-A



PAGE 1-B



RN 169195-92-0 HCAPLUS
CN Benzoic acid, 4-[[4-[[8-[[2,5-dibutoxy-4-[[4-[(1-carboxy-2-mercaptoethyl)amino]-6-[(3-carboxypropyl)amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-2,5-bis(1-methylethoxy)phenyl]azo]- (9CI) (CA INDEX NAME)

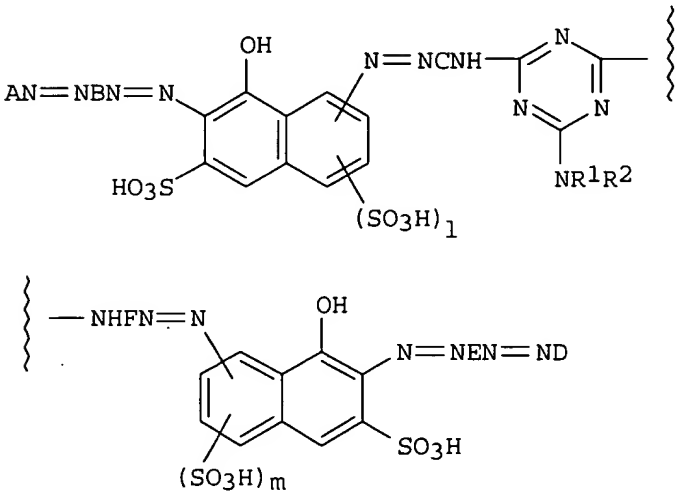


L22 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:804804 HCAPLUS
DOCUMENT NUMBER: 123:343748

TITLE: Recording liquids containing tetraazo dyes
INVENTOR(S): Sano, Hideo; Sato, Nobuyoshi; Murata, Jukichi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07173422	A2	19950711	JP 1993-322244	19931221 <--
PRIORITY APPLN. INFO.:			JP 1993-322244	19931221

OTHER SOURCE(S): MARPAT 123:343748
GI



I

AB Title liqs., useful for ink-jet printing, contain water-based mediums and colorants comprising tetrazo compds., as free acids, I [A, D = (substituted) Ph, naphthyl; B, C, E, F = (substituted) phenylene, naphthylene; R1, R2 = H, C1-18 (substituted) alkyl, C1-18 (substituted) alkenyl, C1-18 (substituted) alkenyl, (substituted) aryl, (substituted) cycloalkyl, (substituted) aralkyl, (substituted) heteocycle; l, m = 0, 1]. Thus, diethylene glycol 10, iso-Pr alc. 3, and tetraazo dye II 3 parts were mixed and blended with balance aqueous NH3 to give 100 parts ink, which was used for ink-jet printing to give images with water resistance and prevention of blurring.

IT **170442-31-6**
RL: TEM (Technical or engineered material use); USES (Uses)
(aqueous ink-jet printing inks containing tetraazo dyes)

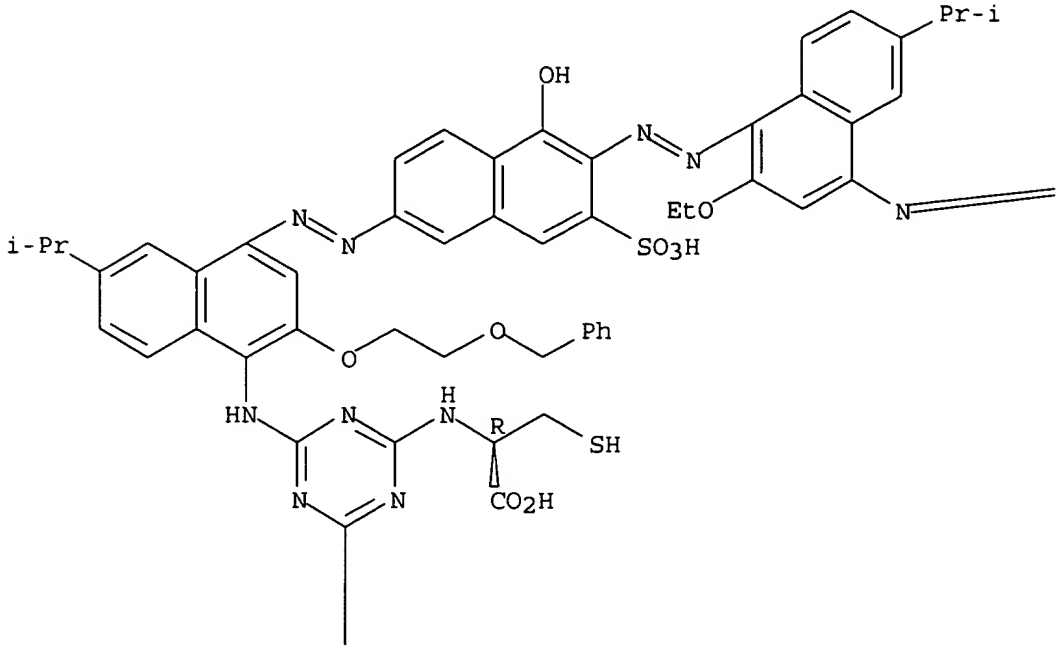
RN 170442-31-6 HCAPLUS

CN L-Cysteine, N-[4-[[4-[[6-[[4-[(4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-6-(1-methylethyl)-1-naphthalenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]azo]-6-(1-methylethyl)-2-[2-(phenylmethoxy)ethoxy]-1-naphthalenyl]amino]-6-[[4-[[6-[[4-[(4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-5-(1-methylethyl)phenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]azo]-5-(1-

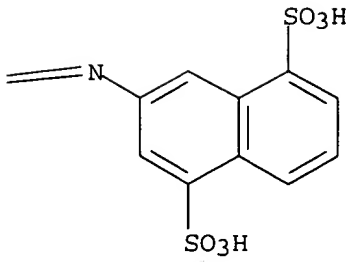
methylethyl)-2-[2-(phenylmethoxy)ethoxy]phenyl]amino]-1,3,5-triazin-2-yl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

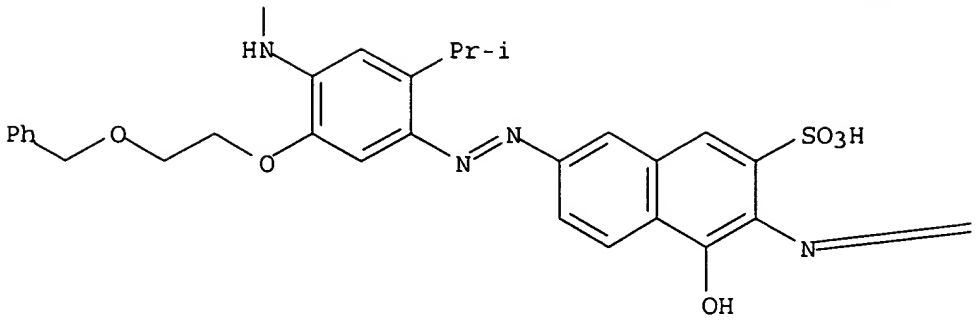
PAGE 1-A



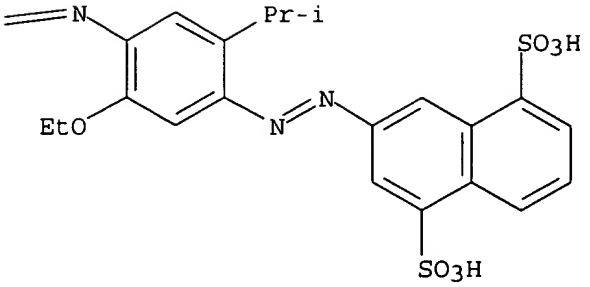
PAGE 1-B



PAGE 2-A



PAGE 2-B



L22 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:785207 HCAPLUS
DOCUMENT NUMBER: 123:343739
TITLE: Water-based recording liquids containing bistriazine-containing tetraazo dyes
INVENTOR(S): Sano, Hideo; Sato, Nobuyoshi; Murata, Jukichi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07150088	A2	19950613	JP 1993-301926	19931201 <--
JP 3511652	B2	20040329		

PRIORITY APPLN. INFO.: JP 1993-301926 19931201
OTHER SOURCE(S): MARPAT 123:343739
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

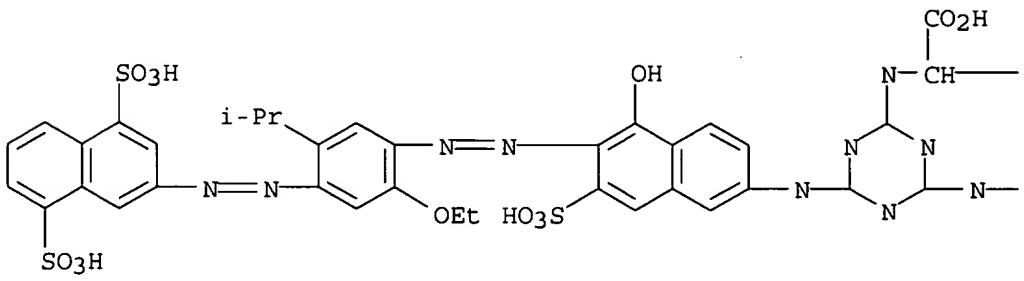
AB Title liqs., useful for ink-jet printer, etc., contain water-based mediums and ≥1 dyes selected from tetraazo compds. I as free acids [A, D = (substituted) Ph, naphthyl; B, C = (substituted) phenylene, naphthylene; R1-4 = H, (substituted) C1-18 alkyl, (substituted) C1-18 alkenyl, (substituted) aryl, (substituted) aralkyl, (substituted) cycloalkyl, (substituted) heterocycle; Y = divalent linking group; m, n = 0, 1]. Thus, diethylene glycol 10, iso-Pr alc. 3, tetrazo dye II 3, and balance water were mixed to give title liquid providing clear bluish black dots in ink-jet printing.

IT **170694-15-2**
RL: TEM (Technical or engineered material use); USES (Uses)
(dyes; inks containing water-based mediums and bistriazine-containing tetraazo
dyes)

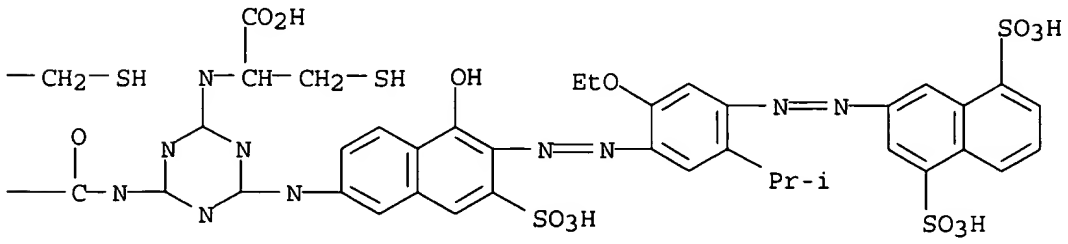
RN 170694-15-2 HCAPLUS

CN L-Cysteine, N,N'-[carbonylbis[imino[6-[[6-[[4-[(4,8-disulfo-2-naphthalenyl)azo]-2-ethoxy-5-(1-methylethyl)phenyl]azo]-5-hydroxy-7-sulfo-2-naphthalenyl]amino]-1,3,5-triazine-4,2-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L22 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:636369 HCAPLUS
DOCUMENT NUMBER: 123:290013
TITLE: Magenta ink solutions containing azo dyes with good

light and water resistance
INVENTOR(S): Sato, Nobuyoshi; Hirasa, Takashi; Murata, Jukichi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 07090212	A2	19950404	JP 1994-178355		19940729 <--
JP 3486966	B2	20040113			
PRIORITY APPLN. INFO.:			JP 1994-178355	A	19940729
			JP 1993-190045		19930730

OTHER SOURCE(S): MARPAT 123:290013
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

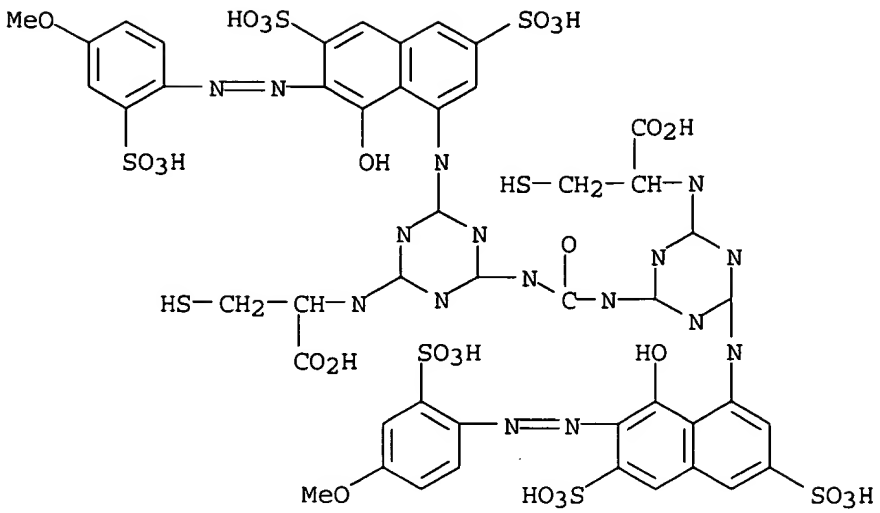
AB The title solns. useful for ink-jet printing, pens, etc., contain, in aqueous medium, azo dyes I [R1-R3, R8-R10 = C1-9 (un)substituted alkyl, C1-9 alkoxy, halogen, H, OH, (un)substituted carbamoyl, (un)substituted sulfamoyl, (un)substituted NH2, NO2, sulfonate ester residue, SO2, carboxylate ester residue; m, n = 0-2; R4-R7 = H, (un)substituted C1-18 alkyl, (un)substituted C1-18 alkenyl, (un)substituted aryl, (un)substituted aralkyl, (un)substituted alicyclyl, (un)substituted heterocyclyl; ≥1 of R4-R7 = 1-4 CO2H-substituted group; Y = divalent group] (as free forms). Thus, an ink containing 3% II was stable at 5 or 60° for 1 mo and provided storage-stable ink-jet prints.

IT **169754-39-6**
RL: TEM (Technical or engineered material use); USES (Uses)
(magenta ink solns. containing azo dyes with good light and water resistance)

RN 169754-39-6 HCAPLUS

CN L-Cysteine, N,N'-[carbonylbis[imino[6-[[8-hydroxy-7-[(4-methoxy-2-sulfophenyl)azo]-3,6-disulfo-1-naphthalenyl]amino]-1,3,5-triazine-4,2-diyl]]]bis-, hexapotassium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

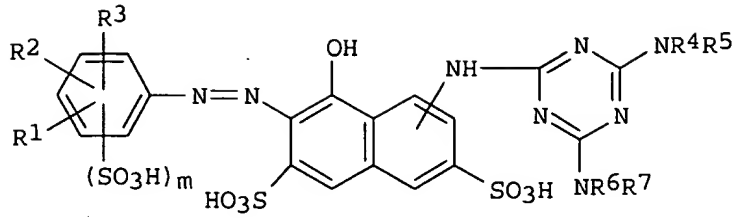
●6 K

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

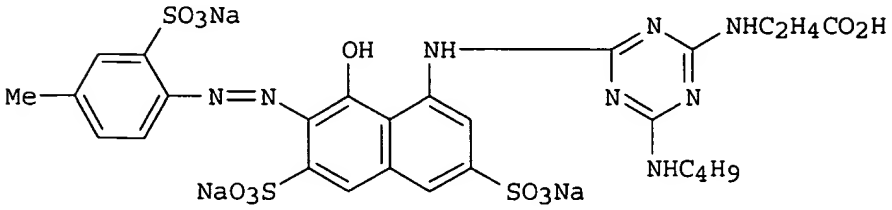
L22 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:636368 HCAPLUS
DOCUMENT NUMBER: 123:290012
TITLE: Magenta ink solutions containing monoazo dyes with good light and water resistance
INVENTOR(S): Sato, Nobuyoshi; Hirasa, Takashi; Murata, Jukichi
PATENT ASSIGNEE(S): Mitsubishi Kagaku KK, Japan; Mitsubishi Chemical Corp.
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 07090211	A2	19950404	JP 1994-146514		19940628 <--
JP 3511677	B2	20040329			
PRIORITY APPLN. INFO.:			JP 1994-146514	A	19940628
			JP 1993-190044		19930730

OTHER SOURCE(S): MARPAT 123:290012
GI



I



II

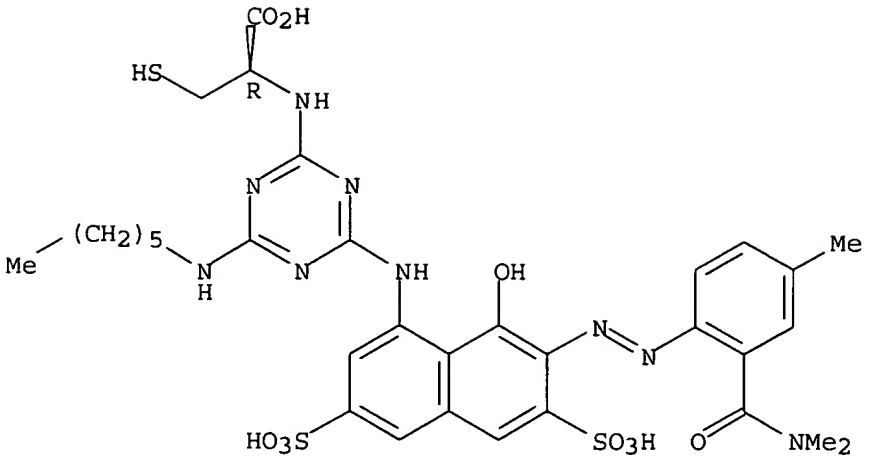
AB The title solns. useful for ink-jet printing, pens, etc., contain, in aqueous medium, monoazo dyes I [R1-R3 = C1-9 (un)substituted alkyl, C1-9 alkoxy, halogen, H, OH, (un)substituted carbamoyl, (un)substituted sulfamoyl, (un)substituted NH2, NO2, sulfonate ester residue, SO2, CO2H, carboxylate ester residue; m = 0-2; R4-R7 = H, (un)substituted C1-18 alkyl, (un)substituted C1-18 alkenyl, (un)substituted aryl, (un)substituted aralkyl, (un)substituted alicyclyl, (un)substituted heterocyclyl; ≥1 of R4-R7 = CO2H-substituted group] in free form. Thus, an ink containing 3% II was stable at 5 or 60° for 1 mo and provided storage-stable ink-jet prints.

IT **169753-83-7**
RL: TEM (Technical or engineered material use); USES (Uses)
(magenta ink solns. containing monoazo dyes with good light and water resistance)

RN 169753-83-7 HCAPLUS

CN L-Cysteine, N-[4-[[7-[[2-[(dimethylamino)carbonyl]-4-methylphenyl]azo]-8-hydroxy-3,6-disulfo-1-naphthalenyl]amino]-6-(hexylamino)-1,3,5-triazin-2-yl]-, dilithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

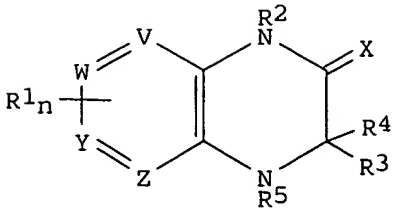


●2 Li

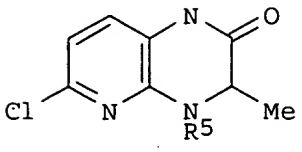
L22 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:700922 HCAPLUS
DOCUMENT NUMBER: 121:300922
TITLE: Preparation of azaquinoxalinones as antiviral agents
INVENTOR(S): Billhardt-Troughton, Uta Maria; Roesner, Manfred; Bender, Rudolf; Meichsner, Christoph
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 42 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 590428	A1	19940406	EP 1993-114934	19930916	<--
EP 590428	B1	19991215			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE					
AT 187724	E	20000115	AT 1993-114934	19930916	
ES 2141744	T3	20000401	ES 1993-114934	19930916	
AU 9347553	A1	19940331	AU 1993-47553	19930923	<--
AU 664643	B2	19951123			
US 5424311	A	19950613	US 1993-125163	19930923	<--
IL 107081	A1	19990714	IL 1993-107081	19930923	
CA 2106882	AA	19940327	CA 1993-2106882	19930924	<--
ZA 9307081	A	19940418	ZA 1993-7081	19930924	<--
HU 65302	A2	19940502	HU 1993-2696	19930924	<--
JP 06211855	A2	19940802	JP 1993-237679	19930924	<--
GR 3032520	T3	20000531	GR 2000-400216	20000131	

PRIORITY APPLN. INFO.: DE 1992-4232392 A 19920926
OTHER SOURCE(S): MARPAT 121:300922
GI



I



II

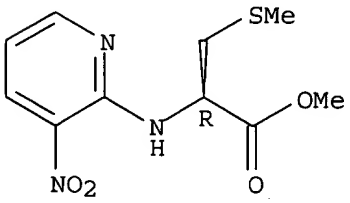
AB Title compds. [tautomeric I; R1 = halo, CF3, OH, (cyclo)alkyl, alkoxy, Ph, etc.; R2,R5 = H, OH, alkyl, etc.; R3,R4 = H, (cyclo)alk(en)yl, (hetero)aryl, etc.; V,W,Y,Z = CH, CR1, N; X = O, S, NR2; n = 0-3] were prepared Thus, 2,6-dichloro-3-nitropyridine was condensed with L-H2NCHMeCO2Me and the reduced monocondensed product cyclized to give title compound (S)-II (R5 = H) which was reductively condensed with Me2CH:CHCHO to give (S)-II (R5 = CH2CH:CHMe2). The latter had MIC of 0.08μg/mL against HIV in cell culture.

IT **159104-71-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiviral agent)

RN 159104-71-9 HCAPLUS

CN L-Cysteine, S-methyl-N-(3-nitro-2-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L22 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:34091 HCAPLUS

DOCUMENT NUMBER: 108:34091

TITLE: Immobilization of urease from Staphylococcus saprophyticus L-1 on activated silicas

AUTHOR(S): Lyubinskii, G. V.; Yanishpol'skii, V. V.; Tertykh, V. A.; Juodvalkite, D.; Glemza, A.

CORPORATE SOURCE: Dep. Chem. Surf., L. V. Pisarzhevsky Inst. Phys. Chem., Kiev, USSR

SOURCE: Ukrainskii Biokhimicheskii Zhurnal (1978-1999) (**1987**), 59(4), 35-41
CODEN: UBZHD4; ISSN: 0201-8470

DOCUMENT TYPE: Journal

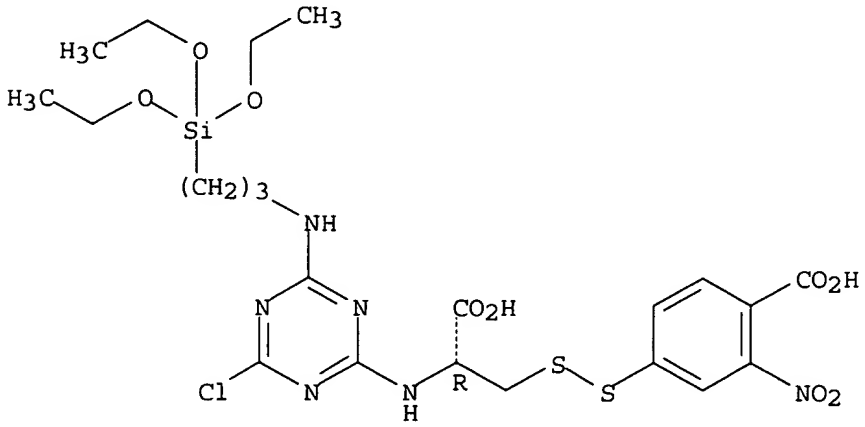
LANGUAGE: Russian

AB The immobilization of urease obtained from S. saprophyticus L-1 on organic silica surfaces was studied. The process completion time (4-5 h) and the optimal pH of binding (7-8) are practically independent of the chemical nature of the carrier surface. The value of the specific activity of urease grafted to silica depends not only on the type of the enzyme-carrier bond, but also on the macromol. protein-to-silica distance. The extent of the retained enzyme activity is 26% after sorption on the

initial silica. It increases to 100% with an increase of the organic radical length which separates the biocatalyst and the carrier.

IT **112147-11-2DP**, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and urease immobilization on)
RN 112147-11-2 HCAPLUS
CN Benzoic acid, 4-[[2-carboxy-2-[[4-chloro-6-[[3-(triethoxysilyl)propyl]amino]-1,3,5-triazin-2-yl]amino]ethyl]dithio]-2-nitro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



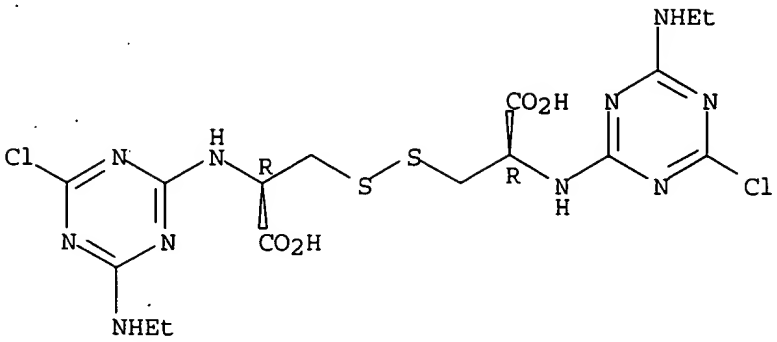
L22 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1986:104256 HCAPLUS
DOCUMENT NUMBER: 104:104256
TITLE: Amino acid conjugates of chloro-s-triazine: model substances for biodegradation study of s-triazine herbicides in plants
AUTHOR(S): Oluic-Vukovic, Vesna; Babic-Gojmerac, Tihomira; Mihanovic, Branka
CORPORATE SOURCE: Fac. Food Sci. Biotechnol., Univ. Zagreb, Zagreb, YU-41000, Yugoslavia
SOURCE: Journal of the Serbian Chemical Society (**1985**), 50(3), 121-4
CODEN: JSCSEN; ISSN: 0352-5139
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To improve the ability to follow the transformation process in plant tissue, 3 amino acid conjugates of chloro-s-triazine were synthesized as model substances and characterized by elemental anal., TLC, IR, and UV spectra. N,N'-Bis(4-chloro-6-ethylamino-s-triazin-2-yl)cystine [**88552-50-5**], one of the model substances, gave bis[β-(6-N-ethylamino-4-hydroxy-s-triazin-2-yl)aminoethyl]disulfide [100595-92-4] upon oxidation with H2O2. Two amino acid conjugates were tested for their herbicidal effect on oats (Avena sativa) in greenhouse expts. Both conjugates exhibited herbicidal activity.

IT **88552-50-5P 100595-91-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and biodegrdn. of, by plants)
RN 88552-50-5 HCAPLUS
CN L-Cystine, N,N'-bis[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI)

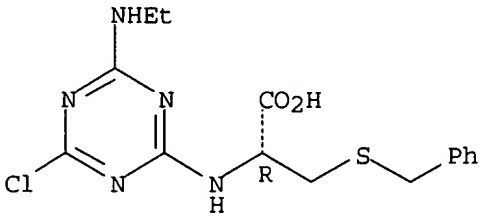
(CA INDEX NAME).

Absolute stereochemistry.

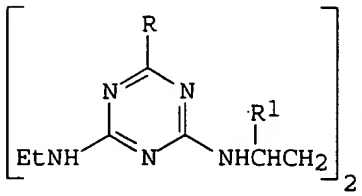


RN 100595-91-3 HCAPLUS
CN L-Cysteine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-S-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:63390 HCAPLUS
DOCUMENT NUMBER: 100:63390
TITLE: Degradation of N,N'-bis(4-chloro-6-ethylamino-S-triazinyl-2)-cystine in buffered extract of cucumber seedlings (Cucumis sativus)
AUTHOR(S): Gojmerac, Tihomira
CORPORATE SOURCE: Fac. Technol., Univ. Zagreb, Zagreb, Yugoslavia
SOURCE: Fragmenta Herbologica Jugoslavica (**1982**), 11(2), 89-97
CODEN: FHJUDA; ISSN: 0350-3615
DOCUMENT TYPE: Journal
LANGUAGE: Serbo-Croatian
GI



I, R=Cl, R^1=CO_2H
II, R=OH, R^1=CO_2H
III, R=OH, R^1=H

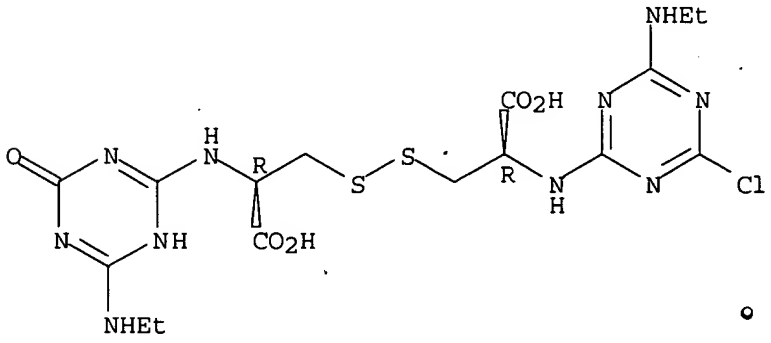
AB Ten-day-old cucumber seedlings were extracted with pH 6.98 phosphate buffer and the extract was incubated with the title triazine-cystine conjugate I [**88552-50-5**] at 4° for 2 wk. The following pathway of I metabolism was determined: I + 2H2O → II [**88552-51-6**] - 2CO2→ III [88552-52-7].

IT **88552-48-1 88552-49-2 88552-51-6**
RL: BIOL (Biological study)
(chloroethylaminotriazinylcystine metabolite in cucumber)

RN 88552-48-1 HCAPLUS

CN L-Cystine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-N'-[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

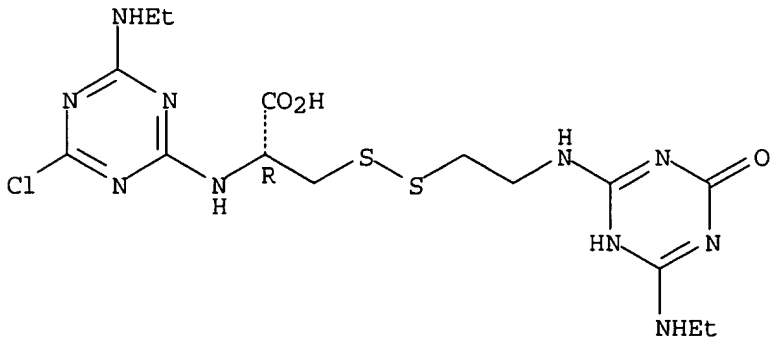
Absolute stereochemistry.



RN 88552-49-2 HCAPLUS

CN L-Alanine, N-[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]-3-[[2-[[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]amino]ethyl]dithio]- (9CI) (CA INDEX NAME)

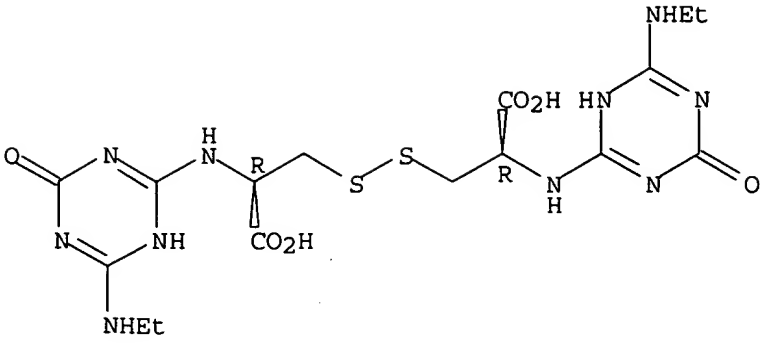
Absolute stereochemistry.



RN 88552-51-6 HCAPLUS

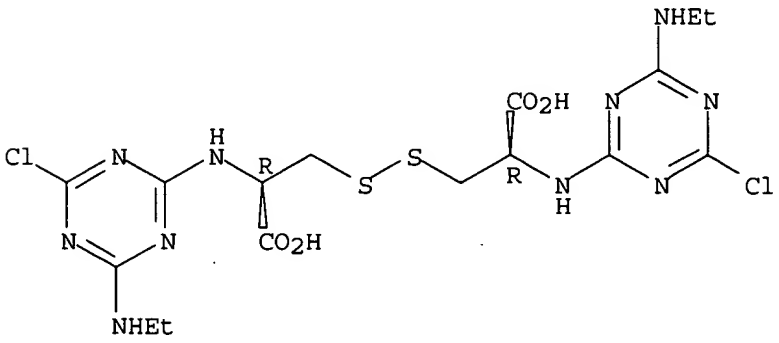
CN L-Cystine, N,N'-bis[6-(ethylamino)-1,4-dihydro-4-oxo-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

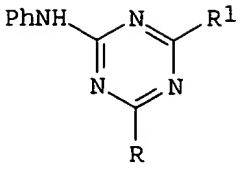


IT **88552-50-5**
RL: PRP (Properties)
(degradation of, by cucumber)
RN 88552-50-5 HCAPLUS
CN L-Cystine, N,N'-bis[4-chloro-6-(ethylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:446607 HCAPLUS
DOCUMENT NUMBER: 93:46607
TITLE: Optically active S-triazine: preparation of α-(2-anilino-4-amino-S-triazin-6-ylamino)-β-thiolpropionic acid
AUTHOR(S): Watanabe, Nobuo; Mitsumoto, Isao; Kato, Tadashi; Usami, Takashi
CORPORATE SOURCE: Tokyo Natl. Tech. Coll., Tokyo, Japan
SOURCE: Tokyo Kogyo Koto Senmon Gakko Kenkyu Hokokusho (**1979**), 11, 83-6
CODEN: TKSHDL; ISSN: 0286-0503
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 93:46607
GI



I

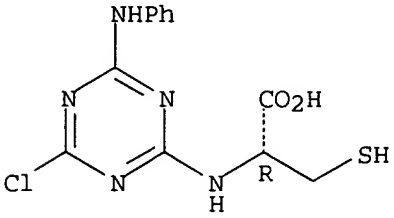
AB The title triazine derivative I [R = NH2, R1 = NHCH(CH2SH)CO2H] was prepared by amination of cyanuric chloride with aniline in acetone at 0-5° to give 96.7% I (R = R1 = Cl)(II), amination of II with L-(-)-cysteine in acetone at 40-50° to give 86.2% I [R = Cl, R1 = NHCH(CH2SH)CO2H], followed by amination with NH4OH 2 h at 80-90°(in 83.3% yield).

IT **74148-69-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

RN 74148-69-9 HCAPLUS

CN L-Cysteine, N-[4-chloro-6-(phenylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

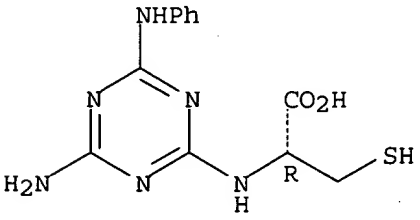


IT **74148-70-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 74148-70-2 HCAPLUS

CN L-Cysteine, N-[4-amino-6-(phenylamino)-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:6900 HCAPLUS
DOCUMENT NUMBER: 92:6900
TITLE: Mononuclear molybdenum(V) complexes of a cysteinyl

peptide
AUTHOR(S): Garner, C. David; Mabbs, Frank E.; Richens, David T.
CORPORATE SOURCE: Chem. Dep., Univ. Manchester, Manchester, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (**1979**), (9), 415-17
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title complexes were prepared by reactions of MoOCl3(THF)2 (I) with a peptide containing cysteinyl and cystinyl groups at .apprx.20°; ESR characteristics and certain chemical behavior observed resemble those of the Mo centers in nitrate reductase and other molybdoenzymes. A mononuclear complex was also obtained by reaction of I with a peptide containing cysteinyl and histidine groups.
IT **72068-28-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ESR of)
RN 72068-28-1 HCAPLUS
CN Molybdenum, trichloro[ethyl N-[(phenylmethoxy)carbonyl]-L-cysteinyl-L-cysteinate bimol. (1→1')-disulfide]oxo-, (OC-6-21)- (9CI) (CA INDEX NAME)

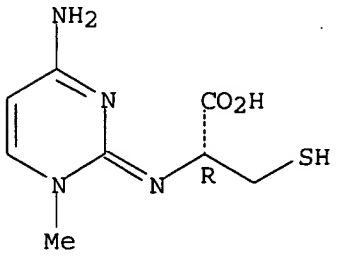
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **72063-46-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72063-46-8 HCAPLUS
CN Molybdenum(1+), dichloro[ethyl N-[(phenylmethoxy)carbonyl]-L-cysteinyl-L-cysteinate bimol. (1→1')-disulfide]dioxo-, (OC-6-22)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L22 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:132899 HCAPLUS
DOCUMENT NUMBER: 88:132899
TITLE: Nucleophilic substitution at C-2 of S-alkylated 2-thiocytidines by cysteine and lysine. A new method for specific covalent linking of peptides to nucleic acids
AUTHOR(S): Kroeger, Manfred; Cramer, Friedrich
CORPORATE SOURCE: Abt. Chem., Max-Planck-Inst. Exp. Med., Goettingen, Fed. Rep. Ger.
SOURCE: Bioorganic Chemistry (**1977**), 6(4), 431-41
CODEN: BOCMBM; ISSN: 0301-4622
DOCUMENT TYPE: Journal
LANGUAGE: English
AB S-alkylated 2-thiocytidine can be substituted at C2 by nucleophilic agents. This reaction was investigated with model compds. as well as with tRNA by using cysteine and lysine to develop a new affinity label linking covalently tRNA and a protein. Reaction with N-protected cysteine gives 2-S-alkylpyrimidines, whereas unprotected cysteine yields an N-alkylpyrimidine after intramol. substitution. With the ε-amino group of lysine a fast replacement at C2 is observed, leading to an unstable 2-N-alkylpyrimidine. All products were characterized chemical and spectroscopically.
IT **66065-59-6P 66065-64-3P**
RL: PREP (Preparation)
(preparation of, nucleate-peptide conjugation in relation to)

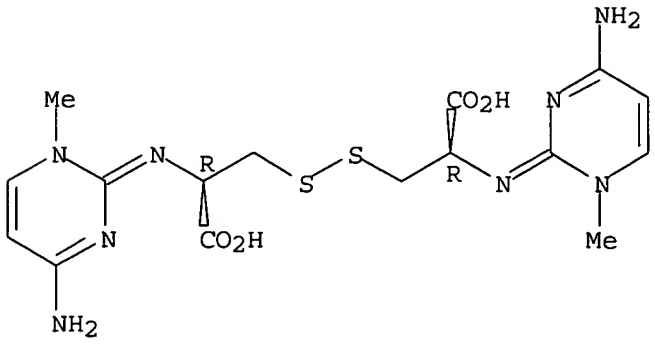
RN 66065-59-6 HCAPLUS
CN L-Cysteine, N-(1,4-dihydro-4-imino-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 66065-64-3 HCAPLUS
CN L-Cystine, N,N'-bis(1,4-dihydro-4-imino-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L22 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:12263 HCAPLUS
DOCUMENT NUMBER: 84:12263
TITLE: Metabolic disposition of carbon-14-labeled azathioprine in the dog
AUTHOR(S): De Miranda, Paulo; Beacham, Lowrie M., III; Creagh, Teresa H.; Elion, Gertrude B.
CORPORATE SOURCE: Wellcome Res. Lab., Burroughs Wellcome Co., Research Triangle Park, NC, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (**1975**), 195(1), 50-7
CODEN: JPETAB; ISSN: 0022-3565
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The metabolic disposition of the methylnitroimidazole moiety of azathioprine (I) [446-86-6], labeled with 14C in carbons 4 and 5 of this imidazole ring, was investigated in the dog. The administration of the radioactive drug (10 mg/kg, orally) was followed, after absorption, by a

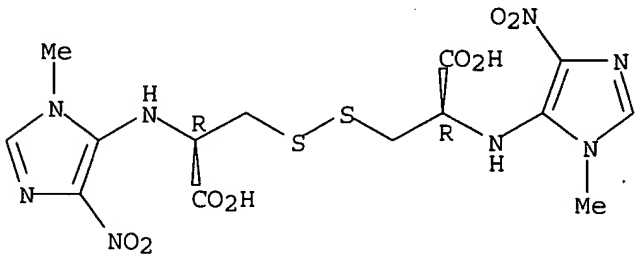
rapid uptake of the radioactivity into the blood cells, with subsequent redistribution to the plasma. The total urinary excretion of 14C was 41.6% in 32 hrs. Anion exchange and high-pressure liquid chromatog. of the urine revealed a large number of 14C-containing metabolites. These included unmetabolized I, 1-methyl-4-nitro-5-(N-acetyl-S-cysteinyl)imidazole [51052-82-5]. 1-Methyl-4-nitro-5-thioimidazole [6339-54-4] and several compds. with ultraviolet absorption spectra similar to 5-substituted amino-1-methyl-4-nitroimidazoles. The most prominent of these was a highly acidic metabolite which was found to be identical in chemical, chromatog. and spectral properties with N,N'-[5-(1-methyl-4-nitro)imidazolyl]cystine [**57350-55-7**]. This metabolite as well as 1-methyl-4-nitro-5-(N-acetyl-S-cysteinyl)imidazole and 1-methyl-4-nitro-5-thioimidazole were also identified in the urine of a dog given 1-methyl-4-nitro-5-(S-glutathionyl)-imidazole [36892-55-4] (10 mg/kg, i.v.) suggesting that the latter compound is an intermediate in the formation of these urinary metabolites. The profile of the methylnitroimidazole urinary metabolites in the dog was similar to that in man and different from that in the rat. A metabolic pathway for the formation of these metabolites in the dog is proposed.

IT **57350-55-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as azathioprine metabolite)

RN 57350-55-7 HCAPLUS

CN L-Cystine, N,N'-bis(1-methyl-4-nitro-1H-imidazol-5-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:564565 HCAPLUS

DOCUMENT NUMBER: 83:164565

TITLE: Methods of peptide sequencing. II. Cyclization of N-2-amino-6-nitrophenyl and N-3-amino-2-pyridyl derivatives of amino acids and peptides

AUTHOR(S): Johnstone, Robert A. W.; Povall, T. Jeffrey; Entwistle, Ian D.

CORPORATE SOURCE: Robert Robinson Lab., Univ. Liverpool, Liverpool, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1975**), (14), 1424-7
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Treatment of amino acid and peptide Me ester hydrochlorides with 2,6-(O2N)2C6H3F on 2-fluoro-3-nitropyridine (I) gave the corresponding N-nitroaryl derivs. Reduction of these derivs. by transfer catalysis and

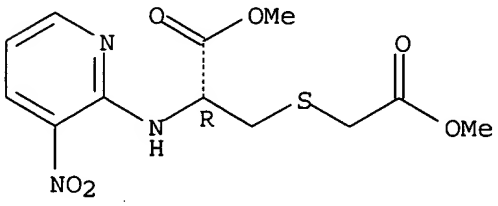
cyclization of the N-aminoaryl derivs. formed gave, in the peptide case, release of the peptide minus its N-terminal amino acid residue. This cycle of reactions was used to obtain a partial sequence of amino acids in a peptide. Thus the hydrochloride of the octapeptide, H-Glu(OMe)-Glu(OMe)-Ala-Glu(OMe)-Glu(OMe)-Ala-Tyr-Gly-OMe on reaction with I gave the corresponding N-nitroaryl derivative which on reduction and cyclization gave initially II, and the corresponding peptide residue. Derivatization and reduction-cyclization steps were repeated with the residue to give successively the pyridopyrazines from Glu(OMe), Ala, and Glu(OMe) twice. At the sixth cycle, no pyridopyrazine corresponding to alanine was detected.

IT **57461-52-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57461-52-6 HCAPLUS

CN L-Cysteine, S-(2-methoxy-2-oxoethyl)-N-(3-nitro-2-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1974:615 HCAPLUS

DOCUMENT NUMBER: 80:615

TITLE: Atrazine metabolism in sorghum. Catabolism of the glutathione conjugate of atrazine

AUTHOR(S): Lamoureux, Gerald L.; Stafford, Lester E.; Shimabukuro, Richard H.; Zaylskie, Richard G.

CORPORATE SOURCE: Metab. Radiat. Res. Lab., Agric. Res. Serv., Fargo, ND, USA

SOURCE: Journal of Agricultural and Food Chemistry (**1973**), 21(6), 1020-30
CODEN: JAFCAU; ISSN: 0021-8561

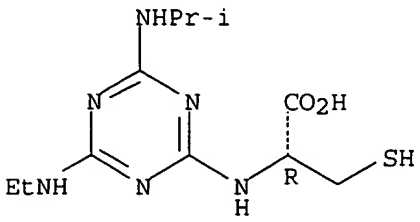
DOCUMENT TYPE: Journal

LANGUAGE: English

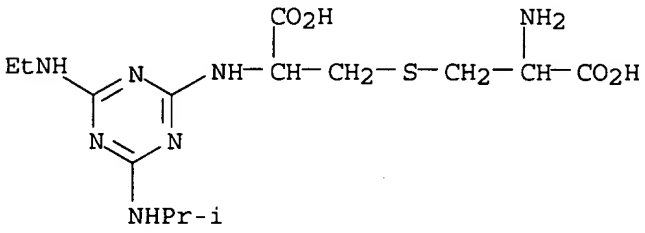
AB The major pathway of atrazine (I) [1912-24-9] metabolism in intact sorghum involved the following steps: I .far. S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)glutathione [24429-05-8] .far. γ-glutamyl-S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine [24428-76-0] .far. S-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine (II) [43171-11-5] .far. N-(4-ethylamino-6-isopropylamino-s-triazinyl-2)cysteine (III) [**43171-12-6**] .far. N-(4-ethylamino-6-isopropylamino-s-triazinyl-2)anthione (IV) [**49564-63-8**]. From 40 to 87% of the I entering sorghum through the roots was metabolized via this pathway. Apparently I could also be metabolized via this route after N-dealkylation. The conversion of II to III was a nonenzymic rearrangement. This was the 1st reported occurrence of II, IV, 2-hydroxy-4-amino-6-isopropylamino-s-triazine [19988-24-0], and 2-hydroxy-4,6-diamino-s-triazine [645-92-1] in sorghum.

IT **43171-12-6 49564-63-8**
RL: FORM (Formation, nonpreparative)
(formation of, as atrazine metabolite in sorghum)
RN 43171-12-6 HCAPLUS
CN L-Cysteine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



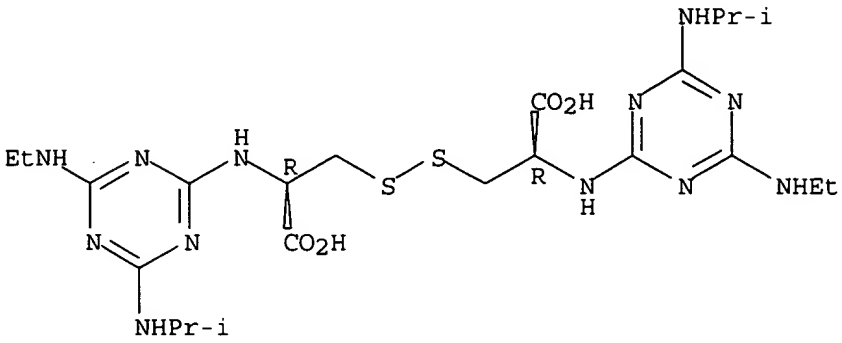
RN 49564-63-8 HCAPLUS
CN L-Cysteine, S-(2-amino-2-carboxyethyl)-N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)



L22 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:543389 HCAPLUS
DOCUMENT NUMBER: 79:143389
TITLE: Atrazine metabolism in sorghum. Chloroform-soluble intermediates in the N-dealkylation and glutathione conjugation pathways
AUTHOR(S): Shimabukuro, Richard H.; Walsh, Wendy C.; Lamoureux, Gerald L.; Stafford, Lester E.
CORPORATE SOURCE: State Univ. Stn., Agric. Res. Serv., Fargo, ND, USA
SOURCE: Journal of Agricultural and Food Chemistry (**1973**), 21(6), 1031-6
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two unrelated metabolites of atrazine (I) [1912-24-9], 2-chloro-4,6-diamino-s-triazine (II) [3397-62-4], and N,N'-bis(4-ethylamino-6-isopropylamino-s-triazinyl-2)cystine (III) [**43171-17-1**], were isolated from sorghum plants treated with 10-5-10-4M I solns. for 5-20 days. II was produced by complete N-dealkylation of I, and no longer inhibited the Hill reaction or cyclic and noncyclic photophosphorylation in isolated pea chloroplasts. The presence of III suggests that I was metabolized by the glutathione pathway to its lanthione conjugate. III is not necessarily present in the plant as the dimer, however the N-cysteine monomer may dimerize in vivo.

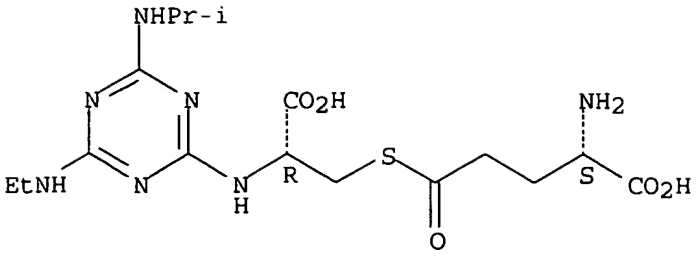
IT **43171-17-1**
RL: BIOL (Biological study)
(as atrazine metabolite, in sorghum)
RN 43171-17-1 HCAPLUS
CN L-Cystine, N,N'-bis[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



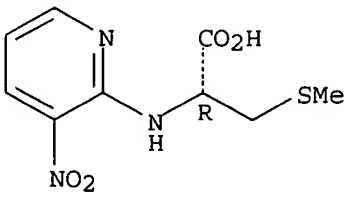
L22 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:415409 HCAPLUS
DOCUMENT NUMBER: 77:15409
TITLE: Metabolism of simazine and atrazine by wild cane
AUTHOR(S): Thompson, Lafayette, Jr.
CORPORATE SOURCE: Dep. Agron., Univ. Kentucky, Lexington, KY, USA
SOURCE: Weed Science (**1972**), 20(2), 153-5
CODEN: WEESA6; ISSN: 0043-1745
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Atrazine (I) [1912-24-9] and simazine (II) [122-34-9] were metabolized in the wild cane (Sorghum bicolor) by hydroxylation and peptide conjugation. The wild cane absorbed in vivo equal amts. of I and II. The plants metabolized 70% of the I and 30% of the II absorbed and translocated to the shoot during 24 hr. The major metabolites formed were hydroxy derivatives and very hydrophilic peptide conjugates, such as S-(4-ethylamino-6-isopropylamino-s-triazin-2-yl)glutathione. The wild cane formed peptide conjugates of I more rapidly than of II, but hydroxylation of I and II occurred at the same rate.
IT **36959-29-2**
RL: FORM (Formation, nonpreparative)
(formation of, in atrazine metabolism by Sorghum bicolor)
RN 36959-29-2 HCAPLUS
CN L-Cysteine, N-[4-(ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]-, 1-hydrogen glutamate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



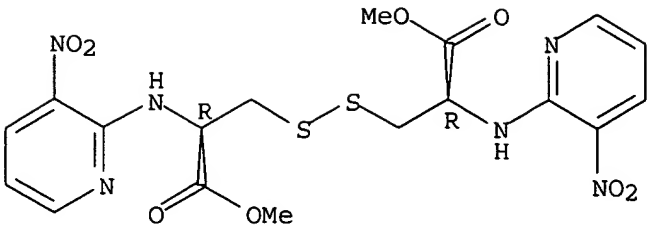
L22 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:405775 HCAPLUS
DOCUMENT NUMBER: 77:5775
TITLE: Nitro heteroaromatic derivatives of amino acids and peptides. III. Application of ultraviolet-visible absorption and circular dichroism to N-(3-nitro-2-pyridyl)amino acids
AUTHOR(S): Toniolo, C.; Nisato, D.; Biondi, L.; Signor, A.
CORPORATE SOURCE: Inst. Org. Chem., Univ. Padova, Padua, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1972**), (9-10), 1179-81
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Uv-visible absorption and CD curves were recorded for 23 N-(3-nitro-2-pyridyl)amino acids, e.g., N-(3-nitro-2-pyridyl)alanine. The 420 nm CD band was correlated with the absolute configuration of N-(3-nitro-2-pyridyl)amino acids, thus allowing determination of the absolute configurations of the N-terminal amino acids of peptides.
IT **36976-96-2 36976-97-3**
RL: PRP (Properties)
(circular dichroism of)
RN 36976-96-2 HCAPLUS
CN L-Cysteine, S-methyl-N-(3-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



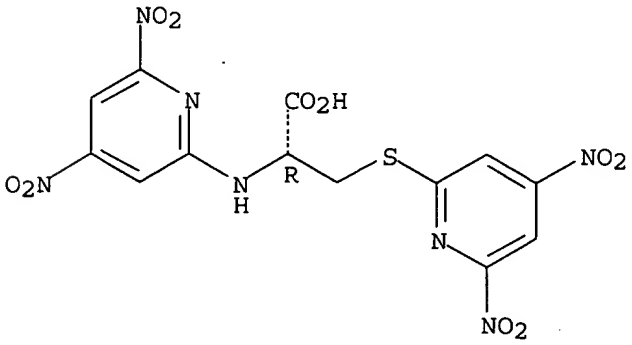
RN 36976-97-3 HCAPLUS
CN L-Cystine, N,N'-bis(3-nitro-2-pyridinyl)-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:141296 HCAPLUS
DOCUMENT NUMBER: 76:141296
TITLE: Nitroheteroaromatic derivatives of amino acids and peptides. II. Optical properties of 3,5-dinitro-2-pyridyl-L-amino acids and related compounds
AUTHOR(S): Nisato, Dino; Marzotto, Armando; De Pieri, Gianfranco; Signor, Angelo
CORPORATE SOURCE: Ist. Chim. Org., Univ. Padova, Padua, Italy
SOURCE: Gazzetta Chimica Italiana (**1971**), 101(11), 805-14
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Amino and pyridyl amino acid derivs., prepared by a coupling reaction of L-amino acids with 2-chloro-3,5-dinitropyridine (I) show a rotation shift varying from 70 to 100° (>300° for proline). Thus, I was added to alanine and Na2CO3 at 40° to give 94% II. Similarly prepared were 3,5-dinitro-2-pyridyl derivs. of arginine, asparagine, aspartic acid, cysteine, glutamine, hydroxyproline, histidine, lysine, phenylalanine, proline, serine, threonine, tryptophan, and glutathione.
IT **35899-61-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35899-61-7 HCAPLUS
CN L-Cysteine, N,S-bis(4,6-dinitro-2-pyridinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



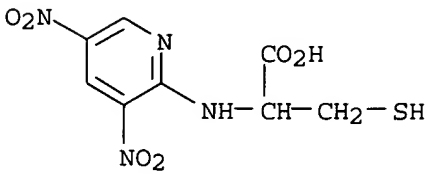
L22 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1968:459052 HCAPLUS
DOCUMENT NUMBER: 69:59052
TITLE: Reactivity of fluoronitropyridines. II. Derivates of fluoronitropyridines
AUTHOR(S): Talik, T.; Talik, Z.
CORPORATE SOURCE: Hochsch. Wirtschaftsfragen, Wroclaw, Pol.
SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (**1968**), 16(1), 7-12
CODEN: BAPCAQ; ISSN: 0001-4095
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Fluoronitropyridines and their derivs. were prepared as previously described (T. Talik and Z. Talik, 1964-7). Their reactivity could be compared as follows: 3,5-dinitro-2-fluoropyridine > 3-fluoro-4-nitropyridine N-oxide > 3-fluoro-5-methyl-4-nitropyridine N-oxide > 2-fluoropyridines with a Me group in the 3, 4, 5, or 6 position and a nitro group in the 3 or 5 position > 3-fluoro-4-nitropyridine > 3-fluoro-2-methyl-4-nitropyridine N-oxide > 2-fluoro-4-nitropyridine > 2,6-dimethyl-3-fluoro-4-nitropyridine N-oxide.

IT **19339-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19339-98-1 HCAPLUS
CN Cysteine, N-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

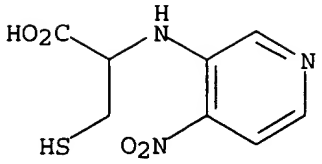


L22 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:459051 HCAPLUS
DOCUMENT NUMBER: 69:59051
TITLE: Reactivity of fluoronitropyridines. III. Conversion of fluoronitropyridines with amino acids
AUTHOR(S): Talik, T.; Talik, Z.
CORPORATE SOURCE: Hochsch. Wirtschaftsfragen, Wroclaw, Pol.
SOURCE: Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques (**1968**), 16(1), 13-16
CODEN: BAPCAQ; ISSN: 0001-4095
DOCUMENT TYPE: Journal
LANGUAGE: German

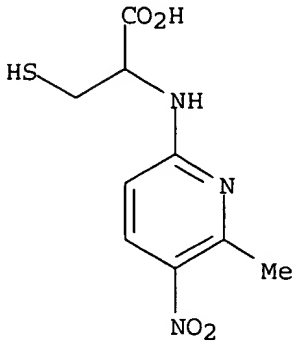
AB 3-Fluoro-4-nitropyridine, its N-oxide and 2-fluoro-5-nitro-6-methylpyridine form crystalline derivs. of the amino acids, which show variable resistance to hydrolysis. They have been used in the quant. study of casein hydrolyzates.

IT **13505-11-8P 18710-42-4P 19367-19-2P**
19367-37-4P 19392-01-9P 19392-17-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13505-11-8 HCAPLUS
CN Cysteine, N-(4-nitro-3-pyridyl)-, DL- (8CI) (CA INDEX NAME)

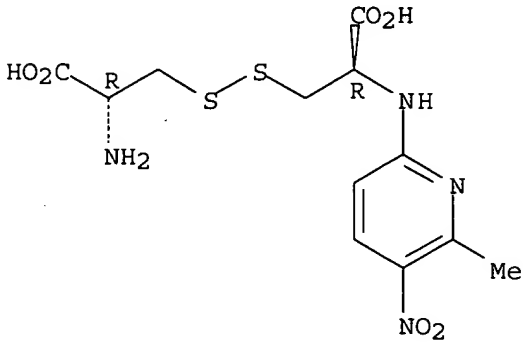


RN 18710-42-4 HCAPLUS
CN Cysteine, N-(6-methyl-5-nitro-2-pyridyl)-, DL- (8CI) (CA INDEX NAME)



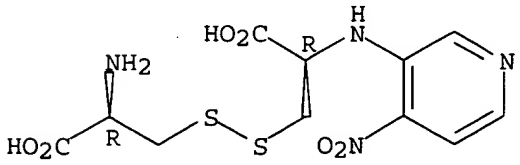
RN 19367-19-2 HCAPLUS
CN Cystine, N-(6-methyl-5-nitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



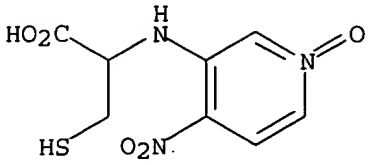
RN 19367-37-4 HCAPLUS
CN Cystine, N-(4-nitro-3-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



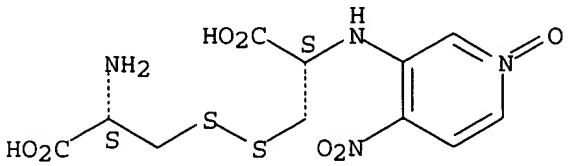
RN 19392-01-9 HCAPLUS

CN Cysteine, N-(4-nitro-3-pyridyl)-, 1-oxide, DL- (8CI) (CA INDEX NAME)



RN 19392-17-7 HCAPLUS
CN Cystine, N-(4-nitro-1-oxido-3-pyridinyl)- (9CI) (CA INDEX NAME)

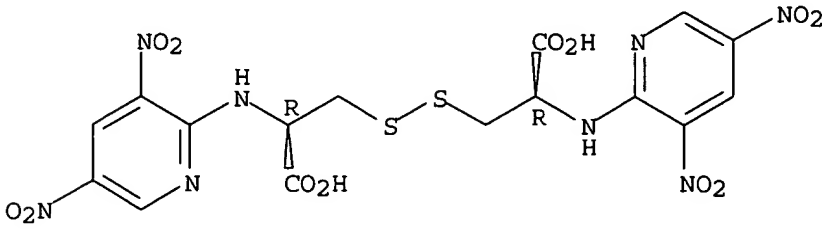
Relative stereochemistry.



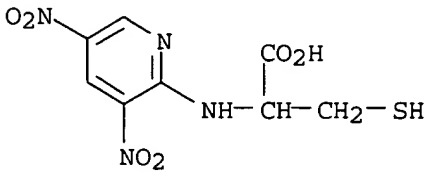
L22 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:410337 HCAPLUS
DOCUMENT NUMBER: 69:10337
TITLE: Synthesis and properties of 2-fluoro-3,5-dinitropyridine
AUTHOR(S): Talik, Tadeusz; Talik, Zofia
CORPORATE SOURCE: Wyzsza Szkola Ekon., Wroclaw, Pol.
SOURCE: Roczniki Chemii (**1967**), 41(9), 1507-11
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB 3,5-Dinitropyridine-2-diazonium fluoroborate (prepared at 0° during 2 hrs. from 75 ml. 48% HF, 35 g. H3BO3, and 6 g. 2-amino-3,5-dinitropyridine, and 9 g. NaNO2) was neutralized with solid (NH4)2CO3 to pH 5 and the whole extracted with Et2O and worked up to give 2.7 g. 2-fluoro-3,5-dinitropyridine (I), m. 64° (C6H6-ligroine). Heating 0.2 g. I 1 min. in 2 ml. H2O led to 2-hydroxy-3,5-dinitropyridine, m. 176°. I refluxed 2 hrs. in MeOH yielded quant. 2-methoxy-3,5-dinitropyridine, m. 92°. Similarly prepared was 2-ethoxy-3,5-dinitropyridine, m. 71°. A mixture of 0.3 g. I, 2 ml. EtOH, and 0.5 g. PhNH2 afforded quant. 2-anilino-3,5-dinitropyridine, m. 152°. Similarly prepared was 2-phenylhydrazino-3,5-dinitropyridine, m. 143°. Heating a mixture of 0.2 g. thiourea and 0.2 g. I in 3 ml. EtOH 2 min., or 0.2 g. I, 0.2 g. MeCSNH2, and 0.2 g. NaHCO3 in 3 ml. EtOH led in both cases to a 50% yield of bis(3,5-dinitro-2-pyridyl) sulfide, m. 164°. A solution of 0.3 g. DL-threonine and 0.42 g. NaHCO3 in 5 ml. H2O was added to 0.47 g. I in 5 ml. EtOH, and the whole kept 5 min. at room temperature, acidified with dilute HCl, and concentrated to give 0.6 g. N-(3,5-dinitro-2-pyridyl)-DL-threonine, m. 121°. Similarly prepared were the following N-(3,5-dinitro-2-pyridyl) amino acid derivs. (amino acid, m.p., and % yield given): L-glutamic, 164°, 89; DL-cysteine,. 159°, 82.9; and L-cystine, 120°, 34.7.
IT **18710-40-2P 19339-98-1P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 18710-40-2 HCAPLUS
CN Cystine, N,N'-bis(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 19339-98-1 HCAPLUS
CN Cysteine, N-(3,5-dinitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

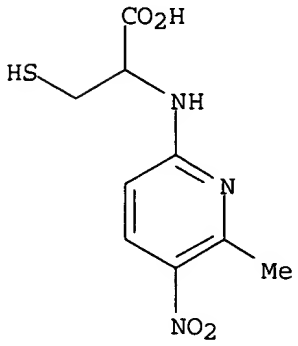


L22 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:403121 HCAPLUS
DOCUMENT NUMBER: 69:3121
TITLE: 2-Fluoro-5-nitro-6-mehtylpyridine. I. Reactions with amino acids
AUTHOR(S): Talik, Zofia; Brekiesz-Lewandowska, Barbara
CORPORATE SOURCE: Wyzsza Szkola Ekon, Wroclaw, Pol.
SOURCE: Roczniki Chemii (**1967**), 41(12), 2095-9
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Syntheses of the title compound (I) and 23 amino acid derivs. were reported. Thus, 10 g. of 2-amino-5-nitro-6-methylpyridine was added at 0° to a solution of 48 g. H3BO3 in 100 ml. 48% HF followed by diazotization 1.5 hrs., with 15 g. solid NaNO2 and the whole stirred 20 min., neutralized with solid NH4HCO3, and steam distilled to give 4 g. I, b5 85°. A mixture of 0.39 g. I, 7 ml. EtOH, 5 ml. H2O, 0.42 g. NaHCO3, and 0.0025 mole of an amino acid refluxed 10 min. until the mixture became clear, was evaporated and acidified with dilute HCl to afford the following N-(5-nitro-6-methyl-2-pyridyl) amino acid derivs. (amino acid, m.p., and % yield given): glycine, 217° (decomposition), 70.4; DL-serine, 169° (decomposition), 56.6; DL-cysteine, 98°, 68.3; DL-α-alanine, 151°, 69.3; β-alanine, 163°, 86.7; DL-asparagine, 187° (decomposition), 72.7; DL-threonine, 170° (decomposition), 61.2; DL-proline, 131°, 77.7; DL-hydroxyproline, 174°, 87.6; DL-glutamic acid, 174°, 69; L-valine, 144°, 84.8; DL-norvaline, 112°, 30.8; DL-methionine, 132°, 60.5; L-histidine, 159°, 40.2;

DL-leucine, 75°, 87.6; DL-isoleucine, 106°, 29.2;
DL-norleucine, 69°, 80.3; DL-lysine, 118°, 76; DL-arginine,
232° (decomposition), 88.3; D-phenylalanine, 90°, 91.6;
L-tyrosine, 204° (decomposition), 73.8; L-tryptophan, 126°, 91.7;
L-cystine, 175° (decomposition), 60.9.

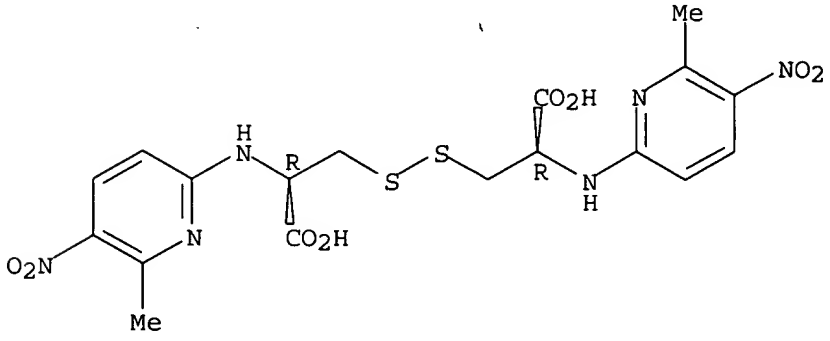
IT **18710-42-4P 18710-61-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 18710-42-4 HCAPLUS
CN Cysteine, N-(6-methyl-5-nitro-2-pyridyl)-, DL- (8CI) (CA INDEX NAME)



RN 18710-61-7 HCAPLUS
CN Cystine, N,N'-bis(6-methyl-5-nitro-2-pyridyl)-, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:11165 HCAPLUS
DOCUMENT NUMBER: 66:11165
TITLE: 3-Fluoro-4-nitropyridine
AUTHOR(S): Talik, Tadeusz; Talik, Zofia
CORPORATE SOURCE: Wyzsza Szkola Ekon., Wroclaw, Pol.
SOURCE: Roczniki Chemii (**1966**), 40(7/8), 1187-93
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: German

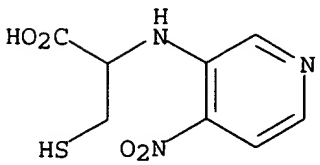
GI For diagram(s), see printed CA Issue.

AB Preparation and reaction of 3-fluoro-4-nitropyridine (I) with amines and amino acids were described. A solution of 5 g. 3-fluoro-4-aminopyridine in 15 ml.

concentrated H_2SO_4 was added at 0° to persulfuric acid (prepared from 60 ml. 20% oleum and 40 ml. 30% H_2O_2), the whole was kept 24 hrs. at room temperature, then poured into ice, neutralized with NH_4HCO_3, and extracted with $CHCl_3$. The extract evaporated and the residue steam distilled gave 4 g. I, b5 62-4°. A solution of 2 g. I in 30 ml. NH_3-saturated MeOH autoclaved 7 hrs. at 130° afforded 1.5 g. 3-amino-4-nitropyridine, m. 140° (H_2O). A solution of 1 g. I and 2 g. $PhNH_2$ in 5 ml. EtOH refluxed 1 hr. yielded 79.2% 3-phenylamino-4-nitropyridine, m. 116° (alc.). Similarly prepared were: 3-ethylamino-4-nitropyridine, m. 96° (H_2O); 3-(ethanolamino) 4-nitropyridine, m. 129° (H_2O). A mixture of 0.5 g. KOH, 4 ml. H_2O, 1 ml. 30% H_2O_2, and 0.5 g. I kept 15 min. until the exothermic reaction ceased and acidified with dilute HCl gave 0.4 g. 3-hydroxy-4-nitropyridine, m. 132° (H_2O). A solution of 1.42 g. I, and MeONa (prepared from 0.23 g. Na and 25 ml. MeOH) kept 1 hr. at room temperature and worked up, yielded 79.5% 3-methoxy-4-nitropyridine, m. 46° (ligroine). Similarly prepared was 89.3% 3-ethoxy-4-nitropyridine, m. 40°. A series of 4-nitro-3-pyridyl amino acid (II) derivs. was prepared according to the following procedure. A solution of 0.005 mole amino acid, 0.01 mole $NaHCO_3$ (or 0.015 mole for dibasic amino acids) in 5 ml. H_2O was stirred with 0.005 mole I in 15 ml. EtOH, then refluxed 15 min. and evaporated in vacuo. The residue acidified with diluted HCl, filtered, and recrystd. afforded the following II (amino acid component, m.p., and % yield given): glycine, 184° (H_2O), 81.2; DL-serine, 196° (H_2O), 44.1; DL-cysteine (III), 154°, 65.8; D,L-α-alanine, 199° (EtOH-H_2O), 70.5; β-alanine, 208° (EtOH-H_2O), 70.5; DL-aspartic acid, 185° (H_2O), 54.9; DL-asparagine (IV), 180° (H_2O), 55.1; DL-threonine, 195° (H_2O), 58.1; DL-proline, 124° (H_2O-EtOH), 75.9; DL-glutamic acid, 162° (H_2O), 59.5; L-glutamine (V), 163° (H_2O), 41; DL-valine, 154° (H_2O-EtOH), 75.3; DL-norvaline, 160° (H_2O-EtOH), 58.6; DL-methionine, 126° (H_2O-EtOH), 59; L-histidine (VI), 242° (H_2O), 50.5; L-leucine, 130° (H_2O-EtOH), 71.1; DL-isoleucine, 184° (H_2O-EtOH), 71.1; DL-norleucine, 147° (H_2O-EtOH), 55.3; L-lysine, 145° (H_2O-EtOH), 52.2; DL-arginine, 219° (H_2O-EtOH), 47.3; D-phenylalanine, 189° (H_2O-EtOH), 55.7; DL-tyrosine, 108° (H_2O-EtOH), 59.4; L-tryptophan (VII), 203°, 89.2; L-cystine, 166° (EtOH), 38. III and VII were purified by dissolving in aqueous Na-HCO_3, shaking with active C, and acidifying with dilute HCl. IV-VI were isolated from the reaction mixture when acidified with HCl at pH 6-7.

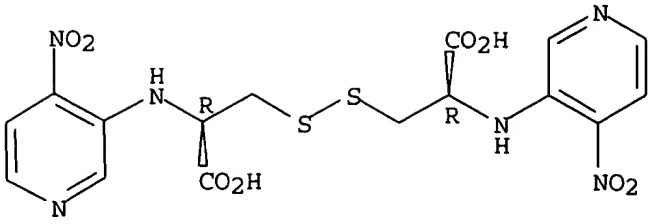
IT **13505-11-8P 15445-33-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13505-11-8 HCAPLUS
CN Cysteine, N-(4-nitro-3-pyridyl)-, DL- (8CI) (CA INDEX NAME)



RN 15445-33-7 HCAPLUS
CN Cystine, N,N'-bis(4-nitro-3-pyridyl)-, L- (8CI) (CA INDEX NAME)

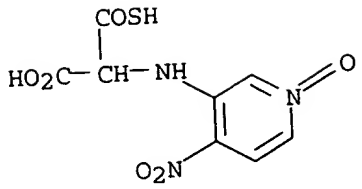
Absolute stereochemistry.



L22 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:461919 HCAPLUS
DOCUMENT NUMBER: 61:61919
ORIGINAL REFERENCE NO.: 61:10769e-h
TITLE: 3-Fluoro-4-nitropyridine N-oxide. II. Reactions with amino acids
AUTHOR(S): Talik, Tadousz; Talik, Zofia
CORPORATE SOURCE: School of Econ., Wroclaw, Pol.
SOURCE: Roczniki Chemii (**1964**), 38(5), 785-8
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Cf. CA 61, 10653c. 3-Fluoro-4-nitropyridine N-oxide (I) readily formed crystalline derivs. with amino acids in high yields. Thus, 0.005 mole of amino acid and 0.01 mole NaHCO3 in 10 ml. H2O warmed at 60° until the solution became clear, treated with a warm (60°) solution of 0.005 mole I in 15 ml. EtOH, kept 10 min. at room temperature, excess alc. evaporated in vacuo, and the residue treated with dilute HCl afforded the crystalline derivative The reaction products of I with lysine, cystine, cysteine, and tryptophan were purified by dissolving in aqueous NaHCO3, stirring with C, and precipitating with dilute HCl. The reaction product of I with histidine was dried in vacuo over P2O5. In the case of dibasic amino acids, 0.015 mole was used. The following addition products of I with the cited amino acid were prepared (m.p., and % yield given): glycine, 216°, 93.9; (±)serine, 212° (decomposition), 52.6; (±)-cysteine, 173° (decomposition), 61.7; (±)-α-alanine, 216° (decomposition), 87.1; β-alanine, 228° (decomposition), 78.4; (±)-aspartic acid, 214° (decomposition), 90.4; (±)-threonine, 203° (decomposition), 54; (±)-proline, 175° (decomposition), 80.8; (±)-glutamic acid, 205° (decomposition), 77.4; (±)-valine, 219° (decomposition), 76.7; (±)-norvaline, 168°, 69; (±)-methionine, 162°, 94.4; (±)-histidine, 199° (decomposition), 84.6; (-)-leucine, 182°,89.2; (±)-isoleucine, 179°,89.2; (±)-norleucine, 164°, 57.8; (±)-lysine, 185° (decomposition), 91.6; (±)-tyrosine, 145° (decomposition), 94.1; (±)-phenylalanine, 202° (decomposition), 99; (±)-tryptophan, 216° (decomposition), 83.5; (±)- cystine, 172° (decomposition), 46.6.

IT **819046-88-3**, Cysteine, N-(4-nitro-3-pyridyl)-, oxide, DL- (preparation of)
RN 819046-88-3 HCAPLUS
CN Cysteine, N-(4-nitro-3-pyridyl)-, oxide, DL- (7CI) (CA INDEX NAME)


COSH
HO2C
CH
NH
N
O
O2N